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Betanidin isomerisation and decarboxylation, thermodynamic and charge transfer dye properties towards dye sensitised solar cells application

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Betanidin isomerisation and decarboxylation, thermodynamic and charge transfer dye properties towards dye sensitised solar cells application

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Abstract

Along with attractiveness of natural dyes for solar technologies, the instability is a well-known drawback of the dyes, which impedes their usage for dye sensitised solar cells (DSSCs) application. The planar isomer appeared to be predominant in equilibrium vapour despite its less energetic stability. Both betanidins belong to red–purple pigments betacyanins, which experimentally demonstrated good adsorption in a visible range. In this study, the structural, thermodynamic, and optoelectronic properties of betanidins have been determined from density functional theory (DFT) and time-dependent DFT (TD–DFT) computations. On the basis of the thermodynamic approach, isomerisation reaction between two structural conformers of betanidin, bent and planar, and also decarboxylation reactions have been analysed. The planar isomer appeared to be predominant in equilibrium vapour despite its less energetic stability; both betanidin molecules exhibit an inclination to decay into decarboxylated betanidin and CO2. As for worthy optoelectronic properties and applicability in DSSCs, the dyes considered satisfy most requirements to sensitise the semiconductor TiO2 and be regenerated by electrolytes. Adsorption of the dyes at the TiO2 surface has been simulated; for the dye@TiO2 complexes, the binding energies, electronic spectra, and relevant molecular orbital (MO) isosurfaces have been computed and discussed.

Keywords

Betanidin; Conformational isomers; Decarboxylated betanidin; DFT; TD–DFT; Thermodynamic and optoelectronic properties